wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 06:11 PM GMT

PDB ID	:	1G63
Title	:	PEPTIDYL-CYSTEINE DECARBOXYLASE EPID
Authors	:	Blaesse, M.; Kupke, T.; Huber, R.; Steinbac, S.
Deposited on	:	2000-11-03
Resolution	:	2.50 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

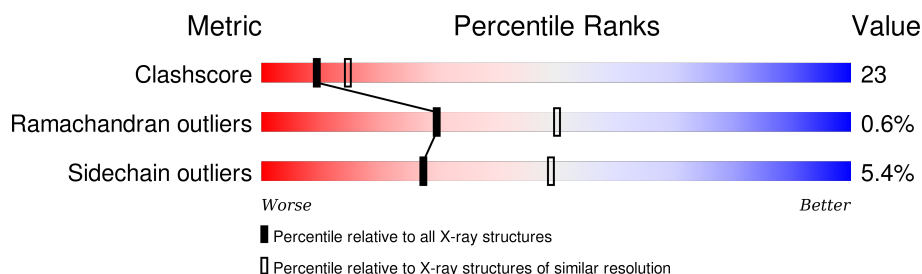|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1   Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Clashscore		23
Ramachandran outliers		0.6%
Sidechain outliers		5.4%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	181	59% 28% • 9%
1	B	181	61% 33% • •
1	C	181	59% 29% • 10%
1	D	181	55% 33% • 10%
1	E	181	55% 32% • 10%
1	F	181	65% 29% • •
1	G	181	54% 34% • 9%

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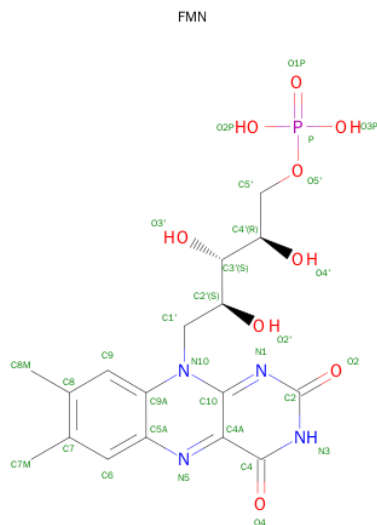| Mol	Chain	Length	Quality of chain
1	H	181	60% 29% 9%
1	I	181	62% 25% 9%
1	J	181	57% 30% 9%
1	K	181	59% 30% 10%
1	L	181	54% 33% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16760 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called EPIDERMIN MODIFYING ENZYME EPID.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total 1321	C 852	N 217	O 243	S 9	0	0	0
1	B	174	Total 1403	C 904	N 231	O 259	S 9	0	0	0
1	C	163	Total 1312	C 846	N 215	O 242	S 9	0	0	0
1	D	162	Total 1304	C 842	N 213	O 240	S 9	0	0	0
1	E	163	Total 1312	C 846	N 215	O 242	S 9	0	0	0
1	F	174	Total 1403	C 904	N 231	O 259	S 9	0	0	0
1	G	164	Total 1321	C 852	N 217	O 243	S 9	0	0	0
1	H	164	Total 1321	C 852	N 217	O 243	S 9	0	0	0
1	I	164	Total 1321	C 852	N 217	O 243	S 9	0	0	0
1	J	164	Total 1321	C 852	N 217	O 243	S 9	0	0	0
1	K	163	Total 1312	C 846	N 215	O 242	S 9	0	0	0
1	L	164	Total 1321	C 852	N 217	O 243	S 9	0	0	0

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	J	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	K	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	L	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	53	Total 53	O 53	0	0
3	B	39	Total 39	O 39	0	0
3	C	28	Total 28	O 28	0	0
3	D	18	Total 18	O 18	0	0
3	E	30	Total 30	O 30	0	0
3	F	29	Total 29	O 29	0	0
3	G	24	Total 24	O 24	0	0
3	H	29	Total 29	O 29	0	0
3	I	30	Total 30	O 30	0	0
3	J	41	Total 41	O 41	0	0
3	K	33	Total 33	O 33	0	0
3	L	62	Total 62	O 62	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
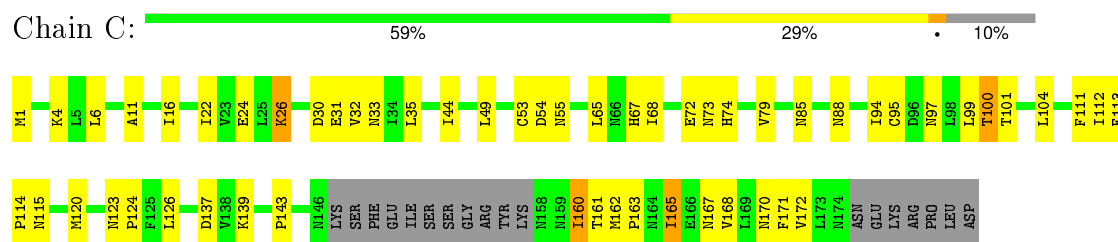
Note EDS was not executed.

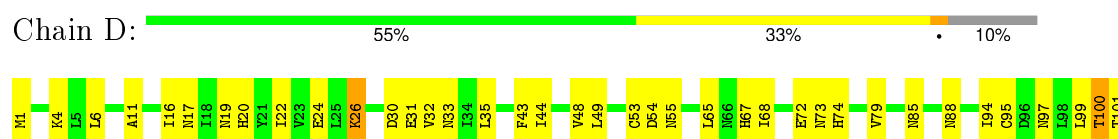- Molecule 1: EPIDERMIN MODIFYING ENZYME EPID
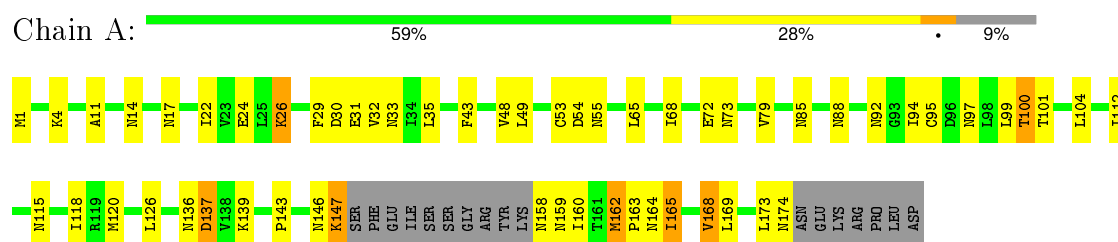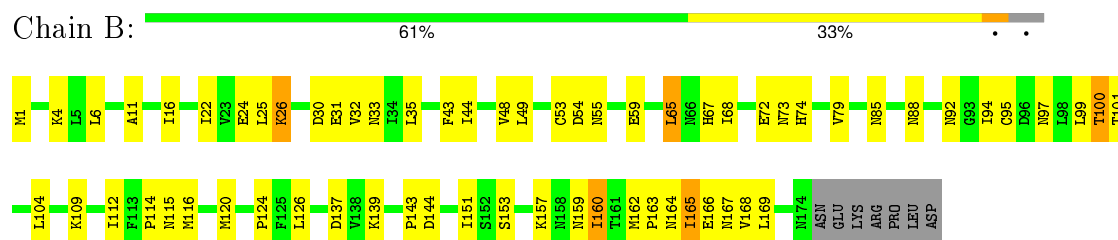
- Molecule 1: EPIDERMIN MODIFYING ENZYME EPID

- Molecule 1: EPIDERMIN MODIFYING ENZYME EPID

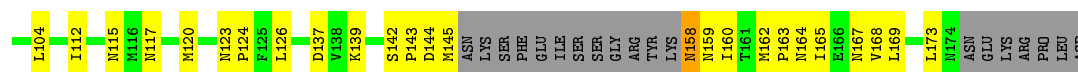- Molecule 1: EPIDERMIN MODIFYING ENZYME EPID

• Molecule 1: EPIDERMIN MODIFYING ENZYME EPID

Chain E:

• Molecule 1: EPIDERMIN MODIFYING ENZYME EPID

Chain F:

• Molecule 1: EPIDERMIN MODIFYING ENZYME EPID

Chain G:

• Molecule 1: EPIDERMIN MODIFYING ENZYME EPID

Chain H:

• Molecule 1: EPIDERMIN MODIFYING ENZYME EPID
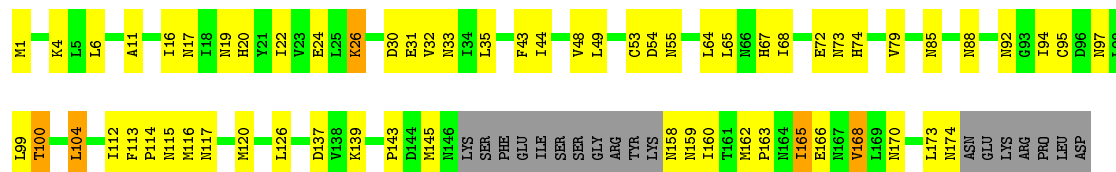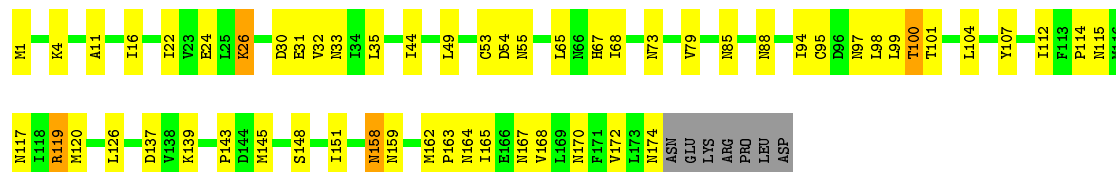
Chain I:

• Molecule 1: EPIDERMIN MODIFYING ENZYME EPID

Chain J:

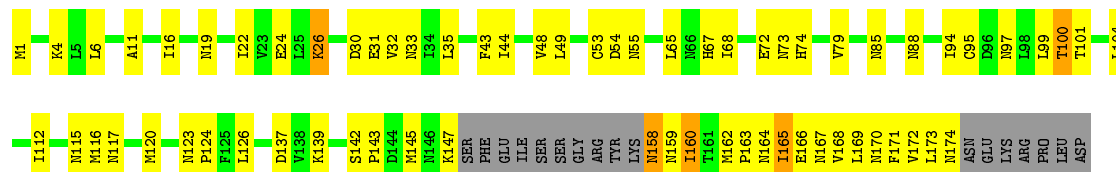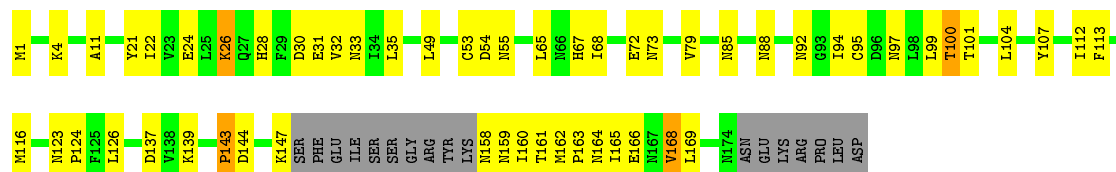• Molecule 1: EPIDERMIN MODIFYING ENZYME EPID

Chain K:

• Molecule 1: EPIDERMIN MODIFYING ENZYME EPID

Chain L:
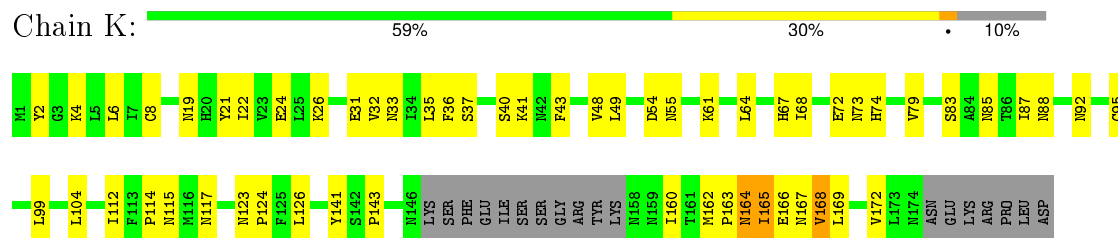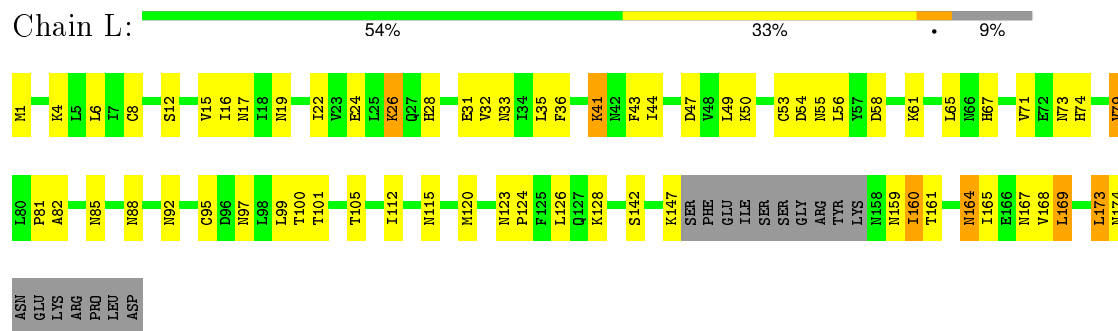
4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	164.68Å 110.03Å 152.87Å 90.00° 90.35° 90.00°	Depositor
Resolution (Å)	14.99 – 2.50	Depositor
% Data completeness (in resolution range)	87.1 (14.99-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	5.80	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.230 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16760	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

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5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FMN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.37	0/1346	0.61	0/1830
1	B	0.38	0/1431	0.61	0/1944
1	C	0.35	0/1337	0.61	0/1819
1	D	0.36	0/1329	0.61	0/1808
1	E	0.36	0/1337	0.61	0/1819
1	F	0.38	0/1431	0.92	3/1944 (0.2%)
1	G	0.36	0/1346	0.60	0/1830
1	H	0.36	0/1346	0.61	0/1830
1	I	0.36	0/1346	0.61	0/1830
1	J	0.43	0/1346	0.66	0/1830
1	K	0.39	0/1337	0.63	0/1819
1	L	0.44	0/1346	0.68	0/1830
All	All	0.38	0/16278	0.65	3/22133 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	119	ARG	NE-CZ-NH2	-21.12	109.74	120.30
1	F	119	ARG	NE-CZ-NH1	19.87	130.24	120.30
1	F	119	ARG	CD-NE-CZ	8.73	135.82	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

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atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1321	0	1337	67	0
1	B	1403	0	1417	76	0
1	C	1312	0	1324	60	0
1	D	1304	0	1318	67	0
1	E	1312	0	1324	69	0
1	F	1403	0	1417	65	0
1	G	1321	0	1337	75	0
1	H	1321	0	1337	68	0
1	I	1321	0	1337	68	0
1	J	1321	0	1337	61	0
1	K	1312	0	1324	69	0
1	L	1321	0	1337	76	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	0	0
2	D	31	0	19	0	0
2	E	31	0	19	0	0
2	F	31	0	19	0	0
2	G	31	0	19	0	0
2	H	31	0	19	0	0
2	I	31	0	19	0	0
2	J	31	0	19	1	0
2	K	31	0	19	0	0
2	L	31	0	19	0	0
3	A	53	0	0	6	0
3	B	39	0	0	4	0
3	C	28	0	0	0	0
3	D	18	0	0	0	0
3	E	30	0	0	0	0
3	F	29	0	0	0	0
3	G	24	0	0	1	0
3	H	29	0	0	1	0
3	I	30	0	0	3	0
3	J	41	0	0	4	0
3	K	33	0	0	1	0
3	L	62	0	0	2	0
All	All	16760	0	16374	741	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 741 close contacts within the same asymmetric unit are listed below, sorted by

their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:CYS:HA	1:C:100:THR:HG23	1.31	1.13
1:F:95:CYS:HA	1:F:100:THR:HG23	1.30	1.12
1:B:95:CYS:HA	1:B:100:THR:HG23	1.29	1.12
1:A:95:CYS:HA	1:A:100:THR:HG23	1.29	1.11
1:G:95:CYS:HA	1:G:100:THR:HG23	1.30	1.10

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	160/181 (88%)	156 (98%)	3 (2%)	1 (1%)	30	50
1	B	172/181 (95%)	168 (98%)	3 (2%)	1 (1%)	30	50
1	C	159/181 (88%)	156 (98%)	2 (1%)	1 (1%)	30	50
1	D	158/181 (87%)	154 (98%)	3 (2%)	1 (1%)	30	50
1	E	159/181 (88%)	154 (97%)	4 (2%)	1 (1%)	30	50
1	F	172/181 (95%)	167 (97%)	4 (2%)	1 (1%)	30	50
1	G	160/181 (88%)	154 (96%)	4 (2%)	2 (1%)	15	26
1	H	160/181 (88%)	154 (96%)	4 (2%)	2 (1%)	15	26
1	I	160/181 (88%)	155 (97%)	4 (2%)	1 (1%)	30	50
1	J	160/181 (88%)	154 (96%)	6 (4%)	0	100	100
1	K	159/181 (88%)	153 (96%)	5 (3%)	1 (1%)	30	50
1	L	160/181 (88%)	156 (98%)	4 (2%)	0	100	100
All	All	1939/2172 (89%)	1881 (97%)	46 (2%)	12 (1%)	30	50

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	160	ILE
1	H	143	PRO
1	H	11	ALA
1	A	11	ALA
1	C	11	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	155/171 (91%)	145 (94%)	10 (6%)	21	39
1	B	164/171 (96%)	155 (94%)	9 (6%)	27	48
1	C	154/171 (90%)	147 (96%)	7 (4%)	34	59
1	D	153/171 (90%)	147 (96%)	6 (4%)	39	66
1	E	154/171 (90%)	143 (93%)	11 (7%)	18	34
1	F	164/171 (96%)	156 (95%)	8 (5%)	31	55
1	G	155/171 (91%)	148 (96%)	7 (4%)	34	59
1	H	155/171 (91%)	149 (96%)	6 (4%)	39	66
1	I	155/171 (91%)	147 (95%)	8 (5%)	29	51
1	J	155/171 (91%)	141 (91%)	14 (9%)	12	22
1	K	154/171 (90%)	151 (98%)	3 (2%)	65	87
1	L	155/171 (91%)	143 (92%)	12 (8%)	16	30
All	All	1873/2052 (91%)	1772 (95%)	101 (5%)	27	49

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	100	THR
1	G	158	ASN
1	L	79	VAL
1	F	119	ARG
1	G	26	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 189 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	88	ASN
1	G	115	ASN
1	L	17	ASN
1	F	129	ASN
1	G	17	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	FMN	A	500	-	32,33,33	1.52	6 (18%)	34,50,50	3.01	8 (23%)
2	FMN	B	501	-	32,33,33	1.63	6 (18%)	34,50,50	2.94	8 (23%)
2	FMN	C	502	-	32,33,33	1.63	6 (18%)	34,50,50	3.00	8 (23%)
2	FMN	D	503	-	32,33,33	1.62	6 (18%)	34,50,50	2.98	8 (23%)
2	FMN	E	504	-	32,33,33	1.66	6 (18%)	34,50,50	2.91	8 (23%)
2	FMN	F	505	-	32,33,33	1.60	6 (18%)	34,50,50	2.97	8 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	FMN	G	506	-	32,33,33	1.65	6 (18%)	34,50,50	2.96	8 (23%)
2	FMN	H	507	-	32,33,33	1.63	6 (18%)	34,50,50	2.98	8 (23%)
2	FMN	I	508	-	32,33,33	1.67	6 (18%)	34,50,50	2.94	8 (23%)
2	FMN	J	509	-	32,33,33	1.60	6 (18%)	34,50,50	3.06	8 (23%)
2	FMN	K	510	-	32,33,33	1.62	7 (21%)	34,50,50	2.98	9 (26%)
2	FMN	L	511	-	32,33,33	1.66	6 (18%)	34,50,50	2.96	8 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	A	500	-	-	0/18/18/18	0/3/3/3
2	FMN	B	501	-	-	0/18/18/18	0/3/3/3
2	FMN	C	502	-	-	0/18/18/18	0/3/3/3
2	FMN	D	503	-	-	0/18/18/18	0/3/3/3
2	FMN	E	504	-	-	0/18/18/18	0/3/3/3
2	FMN	F	505	-	-	0/18/18/18	0/3/3/3
2	FMN	G	506	-	-	0/18/18/18	0/3/3/3
2	FMN	H	507	-	-	0/18/18/18	0/3/3/3
2	FMN	I	508	-	-	0/18/18/18	0/3/3/3
2	FMN	J	509	-	-	0/18/18/18	0/3/3/3
2	FMN	K	510	-	-	0/18/18/18	0/3/3/3
2	FMN	L	511	-	-	0/18/18/18	0/3/3/3

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	510	FMN	O3'-C3'	2.12	1.47	1.43
2	A	500	FMN	C2-N3	2.15	1.42	1.38
2	L	511	FMN	C4-C4A	2.35	1.46	1.41
2	J	509	FMN	C8-C7	2.37	1.47	1.41
2	F	505	FMN	C8-C7	2.40	1.47	1.41

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	505	FMN	C4A-C4-N3	-5.91	115.80	123.52
2	J	509	FMN	C4A-C4-N3	-5.84	115.89	123.52
2	C	502	FMN	C4A-C4-N3	-5.82	115.92	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	511	FMN	C4A-C4-N3	-5.78	115.97	123.52
2	D	503	FMN	C4A-C4-N3	-5.75	116.00	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	509	FMN	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.